



Introduction to ATPESC

Ray Loy
ATPESC Program Director, ANL

Outline



Welcome



Argonne National Laboratory



ATPESC Overview



Logistics



Tour

Welcome!

74 ATPESC 2022 Participants

Àdel	Llibert	Christopher	Brandon	Matthew	Cathrine
Aniruddha	Keith	Michael	Robert	Thomas	Joel
Eloy	Nestor	Akshay	Xiaofeng	Tobias	Donatello
Ke	Arianna	Piyush	Michael	Somdatta	Daniel
Max	Hector	Daniel	Ruixiong	Edward	David
Sergio	Hugo	Willem	Awais	Benjamin	Hannah
Prabhat	Tadbhagya	Sergi	Felix Shiran	Yumeng	Mohammad
Satyajit	Nilesh	Vivek	Manoj	Karl	Gilles
Aviral	Verinder	Juan	Hannah	Vanessa	Shilpa
Saurabh	Olivia	Ashwath	Omkar	Stuart	George
Kaushik	Tien	Kevin	Jialun	Kewei	Tianle
Peter	James	Helen	Naili	Liqui	Hao
Hongyuan	Zhiyong				

Welcome!

ATPESC 2022

51+ Institutions

UC Boulder
ANL
Boston U.
Brown U.
CERN
CMCC
Francis Marion U.
UIUC
KTH Royal Institute of Technology
LLNL
Michigan State U.
NERSC
NCSU
ORNL
Queens U.
Rensselaer Polytechnic Inst.
Stanford U.
U. Jaume I
UCLouvain
UCAR
U. Chicago
U. Connecticut
U. Minnesota
U. Pittsburgh
USC

AFRL
Barcelona Supercomputing Center
BNL
California Inst. of Technology
Environment and Climate Change Canada
Forschungszentrum Jülich GmbH
General Atomics
King's College London
LBNL
U. Alabama Birmingham
NASA Langley
Naval Nuclear Laboratory
Northwestern U.
Politecnico di Milano
Queen Mary U. of London
Rice U.
Texas A&M U.
U. Politècnica de Catalunya
U. Paris-Saclay
UC Santa Cruz
UC Boulder
U. Delaware
U. Ottawa
U. Rochester
Virginia Tech

Argonne National Laboratory

Argonne – a part of DOE National Laboratory System

Office of Science Laboratories

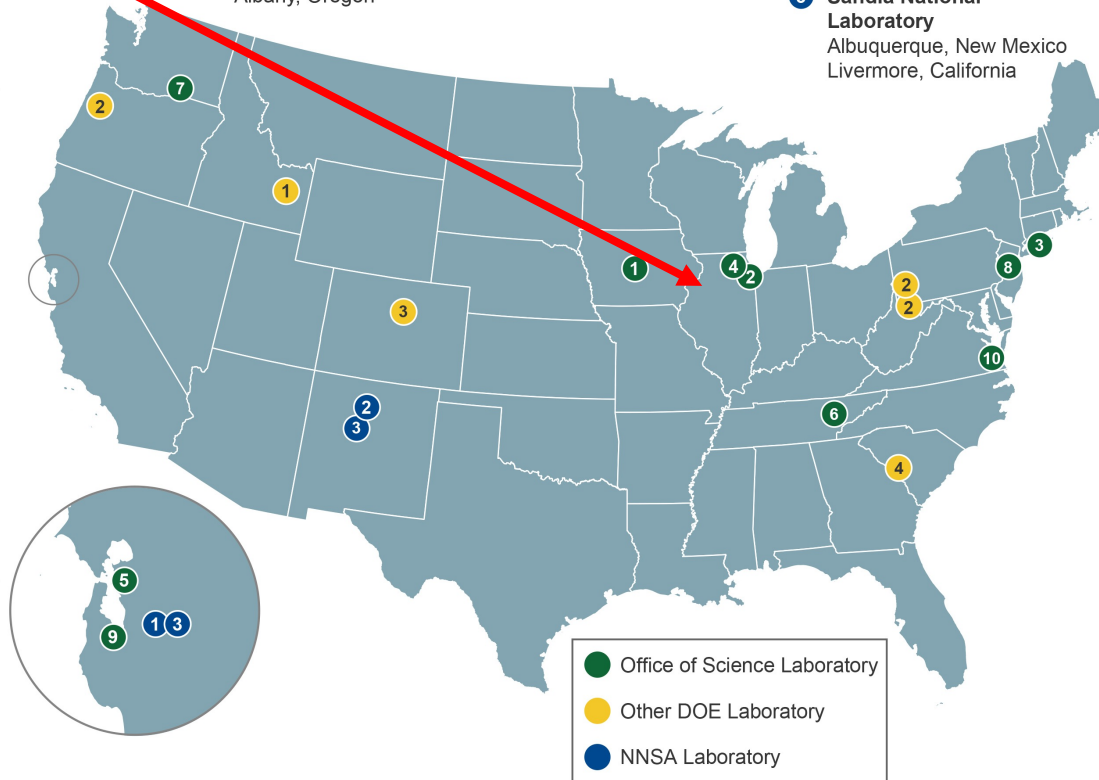
- 1 Ames Laboratory
Ames, Iowa
- 2 Argonne National Laboratory
Argonne, Illinois
- 3 Brookhaven National Laboratory
Upton, New York
- 4 Fermi National Accelerator Laboratory
Batavia, Illinois
- 5 Lawrence Berkeley National Laboratory
Berkeley, California
- 6 Oak Ridge National Laboratory
Oak Ridge, Tennessee
- 7 Pacific Northwest National Laboratory
Richland, Washington
- 8 Princeton Plasma Physics Laboratory
Princeton, New Jersey
- 9 SLAC National Accelerator Laboratory
Menlo Park, California
- 10 Thomas Jefferson National Accelerator Facility
Newport News, Virginia

Other DOE Laboratories

- 1 Idaho National Laboratory
Idaho Falls, Idaho
- 2 National Energy Technology Laboratory
Morgantown, West Virginia
Pittsburgh, Pennsylvania
Albany, Oregon
- 3 National Renewable Energy Laboratory
Golden, Colorado
- 4 Savannah River National Laboratory
Aiken, South Carolina

NNSA Laboratories

- 1 Lawrence Livermore National Laboratory
Livermore, California
- 2 Los Alamos National Laboratory
Los Alamos, New Mexico
- 3 Sandia National Laboratory
Albuquerque, New Mexico
Livermore, California

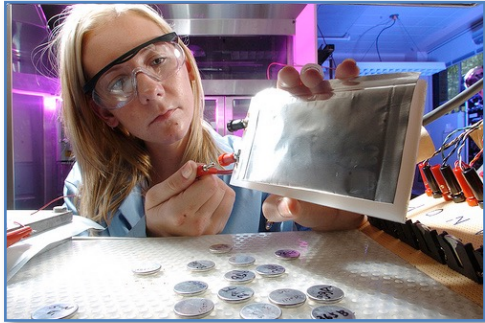


Together, the **17 DOE laboratories** comprise a preeminent federal research system, providing the Nation with strategic scientific and technological capabilities. The laboratories:

- Execute long-term government scientific and technological missions, often with complex security, safety, project management, or other operational challenges;
- Develop unique, often multidisciplinary, scientific capabilities beyond the scope of academic and industrial institutions, to benefit the Nation's researchers and national strategic priorities; and
- Develop and sustain critical scientific and technical capabilities to which the government requires assured access.

[Image Source](#)

Argonne's mission: Provide science-based solutions to pressing



Energy Science



Environmental Sustainability

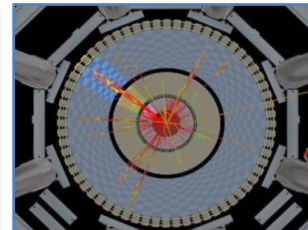
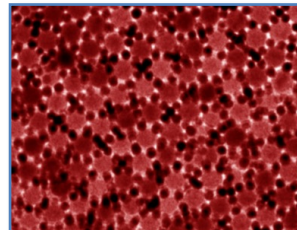


Nuclear and National Security

*Use-Inspired Science and Engineering ...
... Discovery and transformational Science and Engineering*



Major User Facilities



Science and Technology Programs

RESEARCH DIVISIONS

Computing, Environment and Life Sciences

BIO	Biosciences
EVS	Environmental Science
MCS	Mathematics and Computer Science

Energy and Global Security

ES	Energy Systems
GSS	Global Security Sciences
NE	Nuclear Engineering

Photon Sciences

ASD	Accelerator Systems
AES	APS Engineering Support
XSD	X-ray Science

Physical Sciences and Engineering

CSE	Chemical Sciences and Engineering
HEP	High Energy Physics
MSD	Materials Science
NST	Nanoscience and Technology
PHY	Physics

FACILITIES, CENTERS, AND INSTITUTES

User Facilities

APS	Advanced Photon Source
ALCF	Argonne Leadership Computing Facility
ATLAS	Argonne Tandem Linear Accelerator System
ARM	ARM Southern Great Plains
CNM	Center for Nanoscale Materials

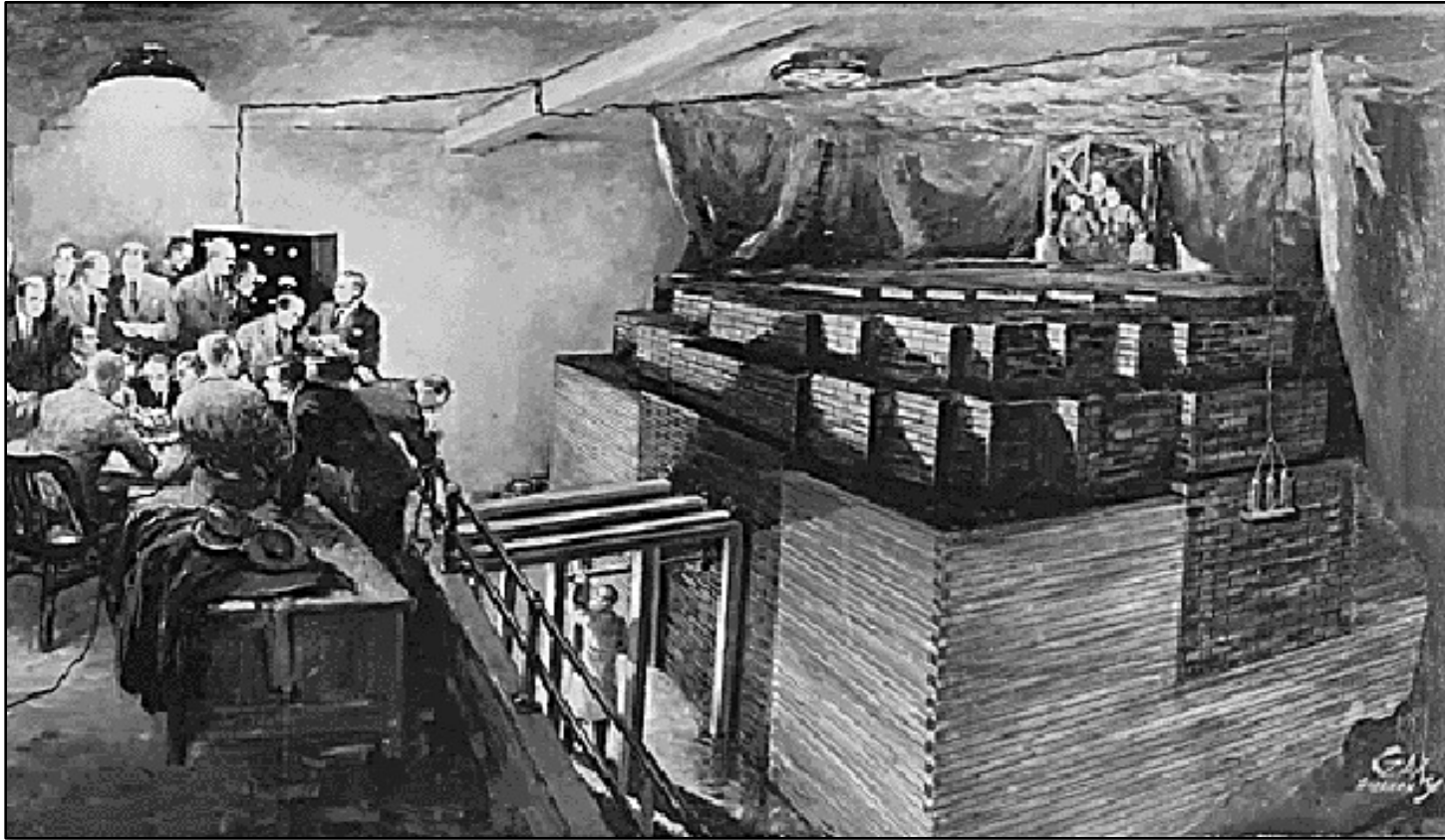
Centers and Joint Institutes

AAI	Argonne Accelerator Institute
ACCESS	Argonne Collaborative Center for Energy Storage Science
ADW	Argonne Design Works
ALI	Argonne Leadership Institute
CEES	Center for Electrochemical Energy Science
CTR	Center for Transportation Research
CRI	Chain Reaction Innovations
CI	Computation Institute
IACT	Institute for Atom-Efficient Chemical Transformations
IGSB	Institute for Genomics and Systems Biology
IME	Institute for Molecular Engineering
JCESR	Joint Center for Energy Storage Research
MCSG	Midwest Center for Structural Genomics
NSP	National Security Programs
NAISE	Northwestern-Argonne Institute for Science and Engineering
RISC	Risk and Infrastructure Science Center
SBC	Structural Biology Center

<https://www.anl.gov>

The origin of Argonne National Laboratory

CP-1 under the bleachers of Stagg field at U. Chicago



Chicago Pile-1 was the world's first artificial nuclear reactor. The first man-made self-sustaining nuclear chain reaction was initiated on December 2, 1942

See also

[*Chicago Pile-1: A Brick History*](#)

Aerial view of Argonne National Laboratory

Advanced
Photon
Source
(APS)

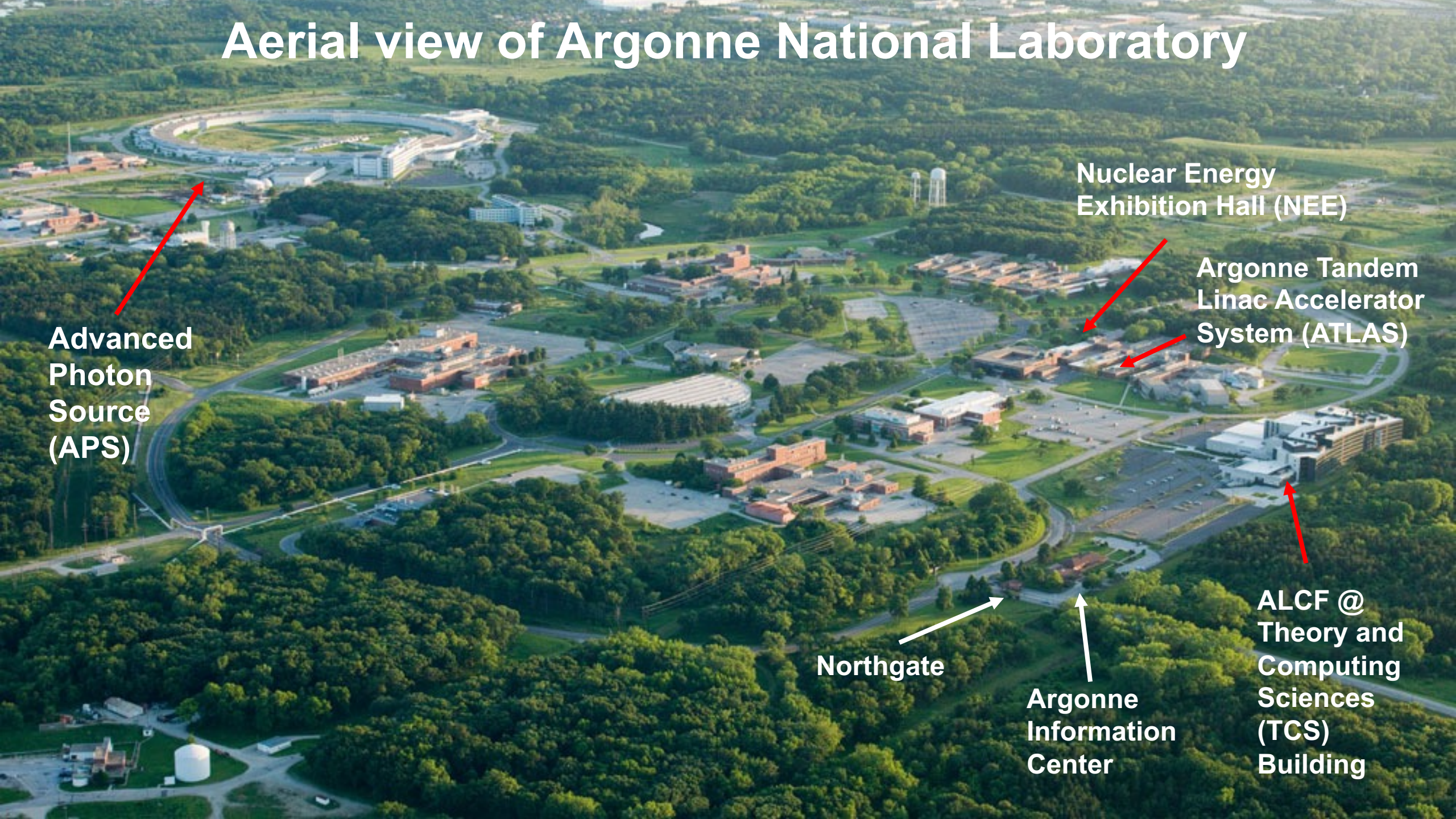
Nuclear Energy
Exhibition Hall (NEE)

Argonne Tandem
Linac Accelerator
System (ATLAS)

ALCF @
Theory and
Computing
Sciences
(TCS)
Building

Northgate

Argonne
Information
Center



Major Scientific User Facilities at Argonne

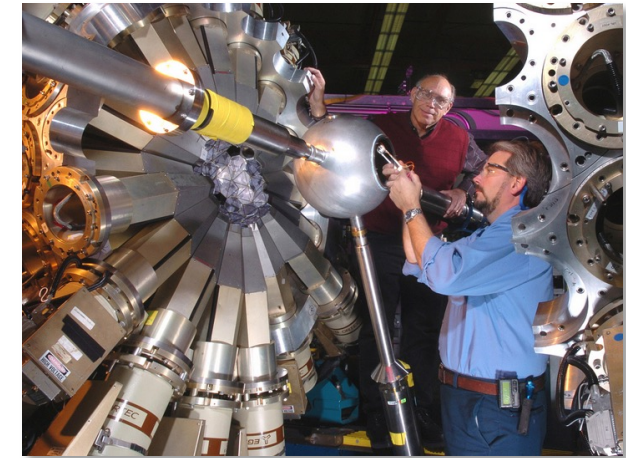
Advanced
Photon
Source



Argonne
Leadership
Computing
Facility

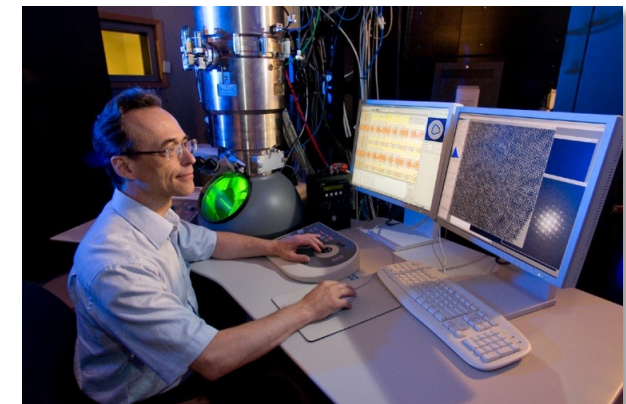


Argonne Tandem Linear
Accelerator System



Center for
Nanoscale
Materials

Electron
Microscopy
Center



AVIDAC (1949-1953)

Argonne's Version of the Institute's Digital Arithmetic Computer



“Moll” Flanders, Director
Jeffrey Chu, Chief Engineer

- **AVIDAC:** based on a prototype at the Institute for Advanced Study in Princeton
- **Margaret Butler wrote AVIDAC's interpretive floating-point arithmetic system**
 - Memory access time: 15 microsec
 - Addition: 10 microsec
 - Multiplication: 1 millisec
- **AVIDAC press release:**
100,000 times as fast as a trained “Computer” using a desk calculator

Early work on computer architecture



Margaret Butler helped assemble the ORACLE computer with ORNL Engineer Rudolph Klein

In 1953...

ORACLE was the world's fastest computer, multiplying 12-digit numbers in .0005 seconds (2Kop/s).

Designed at Argonne, it was constructed at Oak Ridge.

ALCF Timeline

- 2006-2008 BG/L
- 2008-2013 BG/P – Intrepid
- 2012-2019 BG/Q – Mira
- 2017 Theta
- 2022 Polaris
- 2022 Aurora - *Exascale!*



Motivation for ATPESC

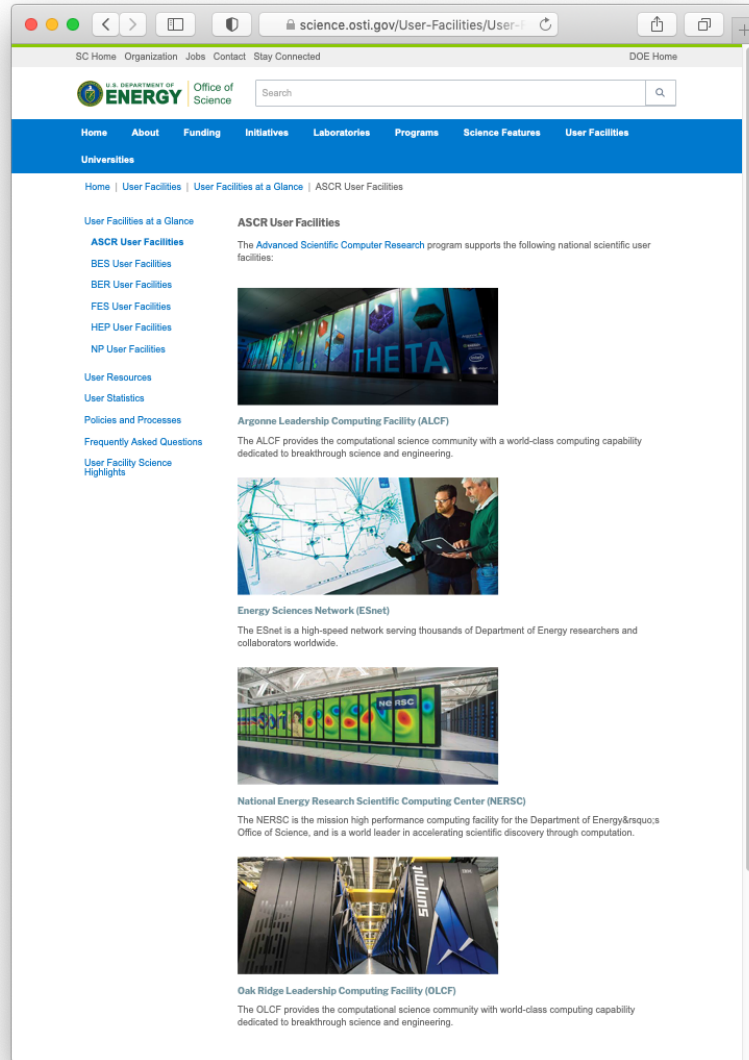
Founded by Paul Messina in 2013. This year is #10 !

- Today's most **powerful supercomputers** have **complex hardware architectures** and **software environments**
 - and even greater complexity is on the horizon on next-generation and exascale systems
- The **scientific and engineering applications** developed for these systems are themselves **complex**
- There is a **critical need for specialized, in-depth training for the computational scientists** poised to facilitate breakthrough science and engineering using these systems

Curriculum Tracks and their leaders

- **Track 1: Hardware Architectures** – Kalyan Kumaran
- **Track 2: Programming Models and Languages** – Rajeev Thakur, Yanfei Guo, Thomas Applencourt
- **Track 3: Data-intensive Computing and I/O** – Rob Latham and Phil Carns
- **Track 4: Visualization and Data Analysis** – Joseph Insley and Silvio Rizzi
- **Track 5: Numerical Algorithms and Software for Extreme-Scale Science** – Lois McInnes, Richard Tran Mills
- **Track 6: Performance Tools and Debuggers**– JaeHyuk Kwack
- **Track 7: Software Productivity and Sustainability** – Anshu Dubey
- **Track 8: Machine Learning and Deep Learning for Science** – Kyle Felker and Sam Foreman

ATPESC Computing Resources



ALCF – Theta, ThetaGPU, Cooley, Polaris,
Sambanova, Cerebras

OLCF – Ascent

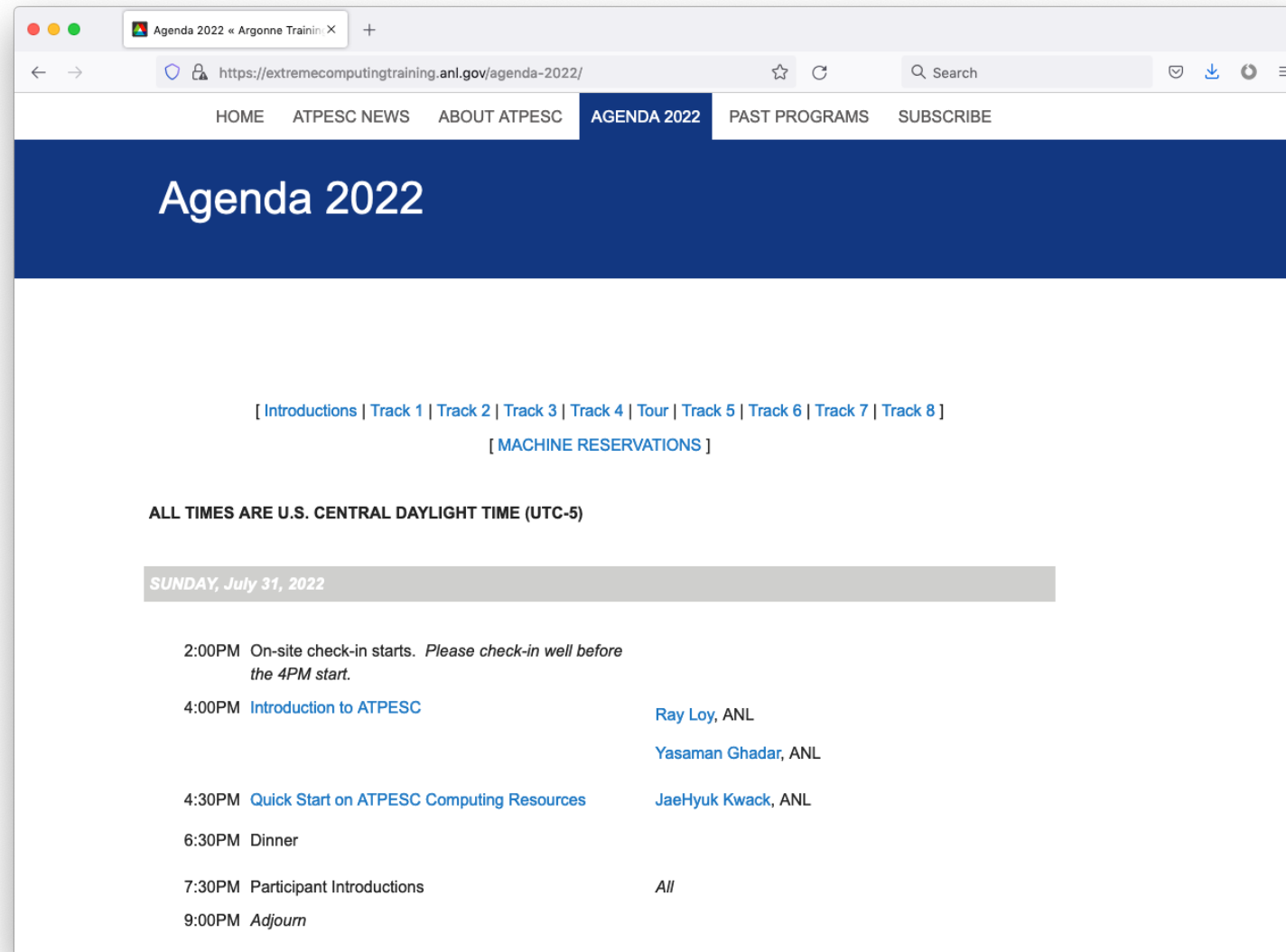
NERSC – general access

Intel Devcloud

AMD Devcloud

<https://science.osti.gov/User-Facilities/User-Facilities-at-a-Glance/ASCR>

<https://extremecomputingtraining.anl.gov/agenda-2022/>



The screenshot shows a web browser window with the URL <https://extremecomputingtraining.anl.gov/agenda-2022/>. The browser's address bar and tabs are visible at the top. The website's navigation menu includes links for HOME, ATPESC NEWS, ABOUT ATPESC, AGENDA 2022 (which is highlighted), PAST PROGRAMS, and SUBSCRIBE. Below the navigation bar is a dark blue header with the text "Agenda 2022" in white. Underneath the header, there are two lines of links: "[Introductions | Track 1 | Track 2 | Track 3 | Track 4 | Tour | Track 5 | Track 6 | Track 7 | Track 8]" and "[MACHINE RESERVATIONS]". A section titled "ALL TIMES ARE U.S. CENTRAL DAYLIGHT TIME (UTC-5)" is followed by a grey bar indicating the date "SUNDAY, July 31, 2022". The agenda for the day is listed below, with times and activities on the left and speakers on the right.

2:00PM	On-site check-in starts. <i>Please check-in well before the 4PM start.</i>	
4:00PM	Introduction to ATPESC	Ray Loy, ANL Yasaman Ghadar, ANL
4:30PM	Quick Start on ATPESC Computing Resources	JaeHyuk Kwack, ANL
6:30PM	Dinner	
7:30PM	Participant Introductions	All
9:00PM	Adjourn	

ATPESC Slack

- alcf-workshops.slack.com
- #announce
- #general for discussion and Q&A during the program
- Topic-related channels (#track-1-hardware)
 - See #announce channel pinned items for a list
 - Or Channels + option to browse
- #help-desk-general
 - Assistance with Zoom or ALCF login issues (see next slide for OLCF and NERSC)
- Please do not DM if you can avoid it
 - You will get help faster via #help-desk-general

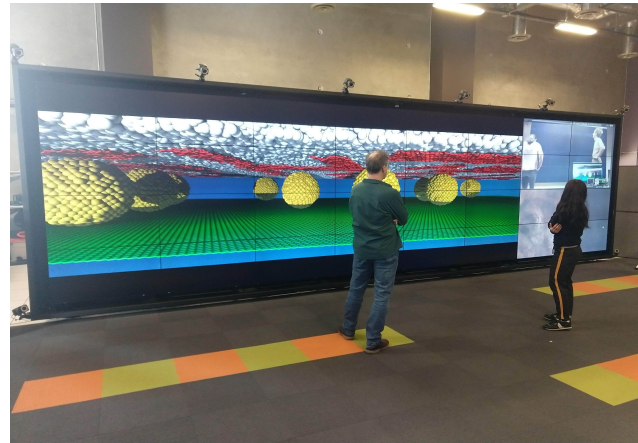
Slack (con't) - Getting help

- ALCF accounts (Theta, ThetaGPU, Cooley)
 - support@alcf.anl.gov (put ATPESC in subject) and slack #help-desk-general
- OLCF accounts
 - Slack #help-desk-olcf-ascent
 - Token issues, call: 865.241.6536 (24x7). Other questions, email: help@olcf.ornl.gov (put ATPESC in subject)
- NERSC accounts
 - accounts@nersc.gov (put ATPESC in subject) or call 1-800-666-3772
- ATPESC general support
 - support@extremecomputingtraining.anl.gov
 - #help-desk-general

Argonne National Laboratory Tour - Livestream

Saturday, August 6, 9AM-11AM – View at St. Charles Amphitheater

- APS – Advanced Photon Source (synchrotron)
- Nuclear Engineering Exhibit
- Main Machine Room in the Theory and Computing Sciences Building (TCS)
- ALCF Visualization Lab



Acknowledgments

Exascale Computing Project



Website: <https://exascaleproject.org>

This training and research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.

ATPESC 2023

- If you or an associate is interested in attending
 - Subscribe to mailing list <https://extremecomputingtraining.anl.gov> (bottom of page)
 - Call for applications usually opens in early January
 - *Read the application instructions carefully*
 - Statement of Purpose and Letter of Recommendation should address how the candidate meets the prerequisites *in detail*.

The future... Aurora Exascale System

